Example 2f: User-Defined Material Properties – USRFUN

This example problem illustrates how the user-defined subroutine, `usrfun.F90`, can be used in conjunction with internal MAC/GMC 4.0 constitutive models to calculate user-defined material properties during execution of the code. The `usrfun.F90` subroutine used in this example is part of the MAC/GMC 4.0 executable. The `usrfun.F90` source code is also distributed with the MAC/GMC 4.0 executable, along with a library file from MAC/GMC 4.0. In order for users to employ their own code to calculate material properties during code execution, it is necessary not only to include the applicable code within the `usrfun.F90` source file, but also to compile the file and link it with the MAC/GMC 4.0 library file. This can be accomplished on a Windows (NT, 2000, XP) PC using the Compaq Visual Fortran software package (v. 6.6) (see http://www.compaq.com/fortran/). For additional information, see the MAC/GMC 4.0 Keywords Manual Introduction (Using User-Defined Subroutines with MAC/GMC 4.0).

It is important to note that in MAC/GMC 4.0, the material properties are associated with constituent materials as opposed to subcells. That is, several subcells may contain material #1, and thus all of those subcells must have the same material properties. This is relevant when employing the `usrfun.F90` subroutine to make material properties a function of field variables, as is done in this example for materials #1 and #2. If, for instance, the properties of material #1 are determined from a function of strain and material #1 is placed in two subcells, the subcells will in general experience different strain states. It is thus impossible for material #1 to have the correct material properties to correspond to the two different states of strain in each subcell. For this reason, when material properties are determined from a function of field variables (other than temperature, which does not vary within the repeating unit cell), each subcell should be given its own material. The present example employs only one subcell, so this is not a problem in this case.

The user-editable portion of the `usrfun.F90` subroutine associated with the three materials examined in this example problem is given in the Appendix. This subroutine is listed in its entirety in the Keywords Manual Appendix. The first material is elastic and has properties that are a function of the axial strain and the previous stiffness. The second material is modeled using incremental plasticity and the post-yield properties are a function of the strain rate. The third material is modeled using the Bodner-Partom viscoplastic constitutive model and the material properties are a function of temperature. The code can be executed for each of these monolithic materials by changing the material number under **`*RUC`**. The thermo-mechanical loading history can also be altered to generate the cases presented in the Results.

MAC/GMC Input File: **`example_2f.mac`**

```
MAC/GMC 4.0 Example 2f - USRFUN Material Properties
*CONSTITUENTS
  NMATS=3
  M=1 CMOD=6  MATID=U MATDB=2
  M=2 CMOD=21 MATID=U MATDB=2
  M=3 CMOD=1  MATID=U MATDB=2
*RUC
# -- Alter value of M=* to change simulated material
  MOD=1 M=1
*MECH
  LOP=1
```

```
# -- Alter values of TI=* to change simulated rate
#    Example: use TI=0.,2000. for rate = 0.00001/sec.
  NPT=2 TI=0.,200. MAG=0.,0.02 MODE=1
*THERM
# -- Alter values of TI=* to change simulated rate
# -- Alter values of TEMP=* to change simulated temperature
  NPT=2 TI=0.,200. TEMP=23.,23.
*SOLVER
# -- Alter values of TI=* (and STP=*) to change simulated rate
  METHOD=1 NPT=2 TI=0.,200. STP=1. ITMAX=50 ERR=1.E-6
*PRINT
  NPL=6
*XYPLOT
  FREQ=1
  MACRO=1
   NAME=example_2f X=1 Y=7
  MICRO=0
*END
```

Annotated Input Data

1) Flags: None

2) Constituent materials (***CONSTITUENTS**) [KM_2]:

Number of materials:	3	(NMATS=3)
Constitutive models:	Linearly elastic	(CMOD=6)
	Incremental plasticity	(CMOD=21)
	Bodner-Partom viscoplasticity	(CMOD=1)
Materials:	User-defined	(MATID=U)
Material property source:	`usrfun.F90` subroutine	(MATDB=2)

3) Analysis type (***RUC**) → Repeating Unit Cell Analysis [KM_3]:

Analysis model:	Monolithic material	(MOD=1)
Material assignment:	Each constituent successively	(M=*)

4) Loading:

a) Mechanical (***MECH**) [KM_4]:

Loading option:	1	(LOP=1)
Number of points:	2	(NPT=2)
Time points:	0., 200. sec.	(TI=0.,200.)
Load magnitude:	0., 0.02	(MAG=0.,0.02)
Loading mode:	strain control	(MODE=1)

To alter the strain rate as is done to generate Figure 2.8, the second time point can be changed. For example, to increase the applied strain rate from 0.0001 /sec. to 0.001 /sec., use `TI=0.,20.`.

b) Thermal (***THERM**) [KM_4]:

Number of points:	2	(NPT=2)
Time points:	0., 200. sec.	(TI=0.,200.)
Temperature points:	23., 23.	(TEMP=23.,23.)

☞ Note: The ending time point should match up with that given in ***MECH**. Also, to alter the temperature as is done to generate Figure 2.9, both temperature values (`TEMP=*,*`) should be changed.

c) Time integration (***SOLVER**) [KM_4]:

Time integration method:	Forward Euler	(`METHOD=1`)
Number of time points:	2	(`NPT=2`)
Time points:	0., 200. sec.	(`TI=0.,200.`)
Time step sizes:	0.1 sec.	(`STP=0.1`)
Max. number of iterations	50	(`ITMAX=50`)
Max. permitted error fraction	$1.\times10^{-6}$	(`ERR=1.E-6`)

☞ Note: While `ITMAX=50` and `ERR=1.E-6` are present in the input file for all cases executed in this example problem, these data are required only for the incremental plasticity cases. Also, as was the case in ***THERM**, the ending time point must be altered to match that employed in ***MECH**. Also, as the total time for the simulation is altered, as in Figure 2.8, the time step size can be changed accordingly so that the total number of time steps remains constant.

5) Damage and Failure: None

6) Output:

a) Output file print level (***PRINT**) [KM_6]:

Print level:	6	(`NPL=6`)

b) x-y plots (***XYPLOT**) [KM_6]:

Frequency:	1	(`FREQ=1`)
Number of macro plots:	1	(`MACRO=1`)
Macro plot name:	example_2f	(`NAME=example_2f`)
Macro plot x-y quantities:	ε_{11}, σ_{11}	(`X=1 Y=7`)
Number of micro plots:	0	(`MICRO=0`)

7) End of file keyword: (***END**)

Results

Results in the form of simulated stress-strain curves are given in Figure 2.7, Figure 2.8, and Figure 2.9. It is important to remember that these results have been generated based on the version of the `ursfun.F90` subroutine that is distributed with MAC/GMC 4.0. This version of the subroutine is contained within the distributed MAC/GMC 4.0 executable. However, if the `usrfun.F90` subroutine source code is altered and compiled and linked to the MAC/GMC 4.0 library file, this example problem may not execute as expected.

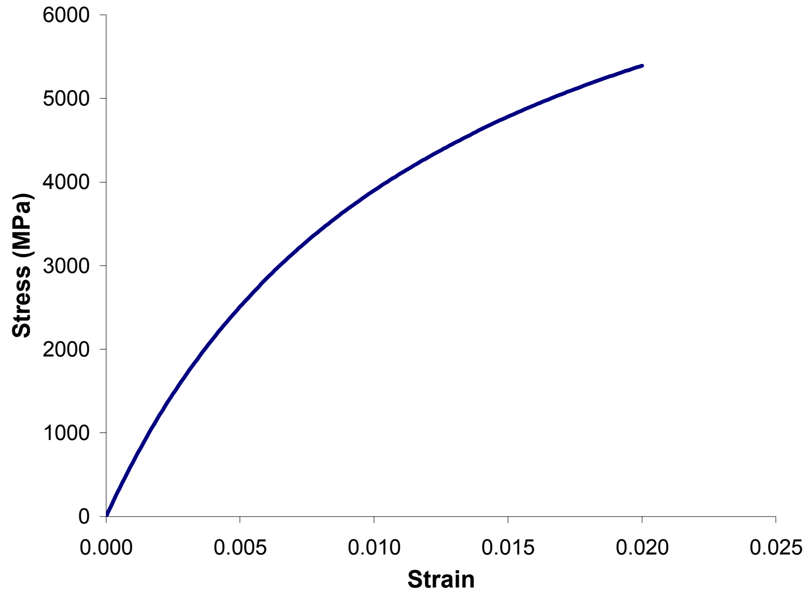

Figure 2.7 Example 2f: plot of the tensile stress-strain response for material #1 – elastic material with stiffness a function of strain and previous stiffness.

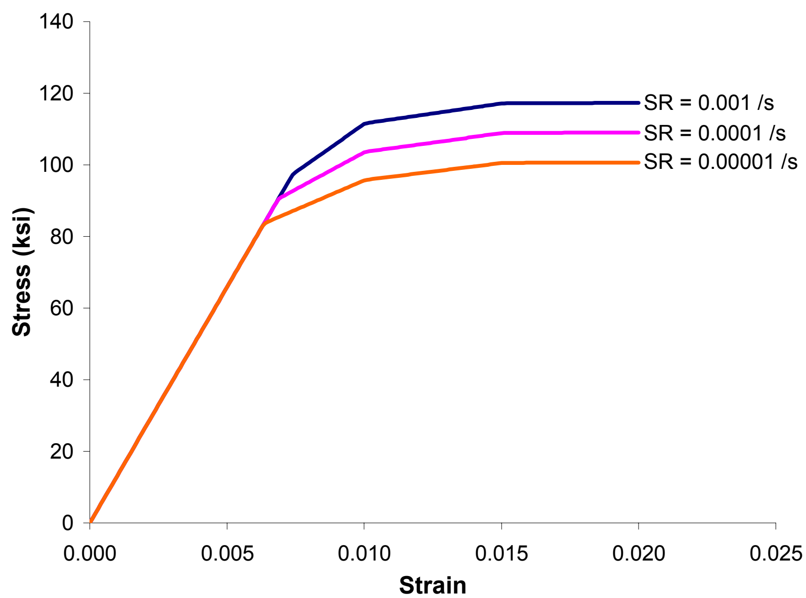

Figure 2.8 Example 2f: plots of the tensile stress-strain response for material #2 – point-wise incremental plasticity material with post-yield behavior a function of strain rate.

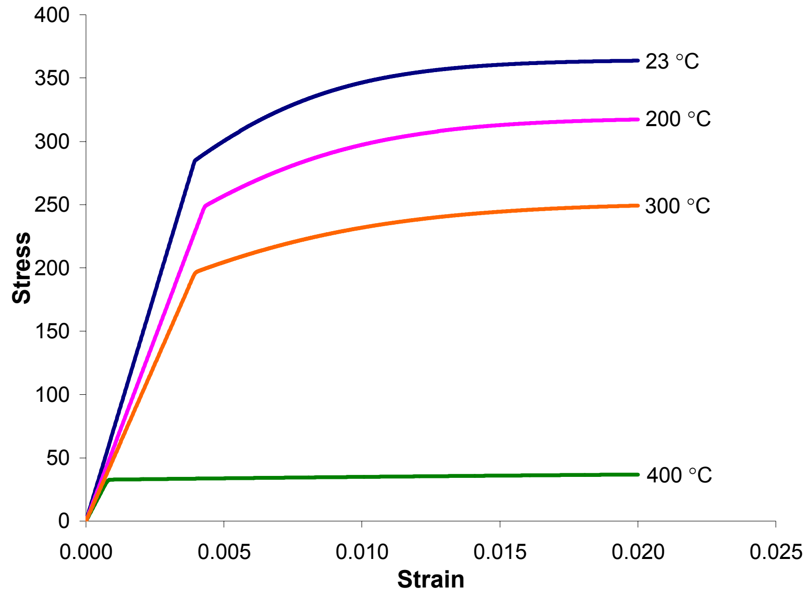

Figure 2.9 Example 2f: plots of the tensile stress-strain response for material #3 – Bodner-Partom viscoplastic material with elastic and viscoplastic material properties a function of temperature.